

trans-1-(Isopropylthio)-2-butene

Inchi:	InChI=1S/C7H14S/c1-4-5-6-8-7(2)3/h4-5,7H,6H2,1-3H3/b5-4+
InchiKey:	NBTBAEQTCSNSGX-SNAWJCMRSA-N
Formula:	C7H14S
SMILES:	CC=CCSC(C)C
Mol. weight [g/mol]:	130.25
CAS:	88916-22-7

Physical Properties

Property code	Value	Unit	Source
gf	118.96	kJ/mol	Joback Method
hf	-34.00	kJ/mol	Joback Method
hfus	14.70	kJ/mol	Joback Method
hvap	37.56	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.704		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
tb	432.06	K	Joback Method
tc	633.55	K	Joback Method
tf	182.97	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.01	J/mol×K	432.06	Joback Method
cpg	242.83	J/mol×K	465.64	Joback Method
cpg	255.04	J/mol×K	499.22	Joback Method
cpg	266.64	J/mol×K	532.80	Joback Method
cpg	277.66	J/mol×K	566.38	Joback Method
cpg	288.11	J/mol×K	599.97	Joback Method
cpg	298.03	J/mol×K	633.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88916227&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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